Second Cross Virial Coefficients for Interactions Involving Water: Compilation and Correlation of Data

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Values of the second cross virial coefficients (B) and cross Joule-Thomson coefficients for interactions involving water are compiled or evaluated from existing experimental data (PVT properties and excess enthalpies of gas mixtures, solubility of the condensed phases of liquid water or ice in compressed gases). In all there are data for interactions between water and 29 other compounds, including simple fluids (inert gases, methane, nitrogen), nonpolar (alkanes), polar (chloromethane, for example), and "hydrogen-bonding" (methanol, ammonia) compounds, i.e. interactions covering the whole range of forces operating between water and nonelectrolyte solutes. These values of the second cross virial coefficients are typically available over a limited temperature range, and the quality of data for most interactions does not allow a meaningful parameterization of even simple intermolecular potential energy functions. However, it is possible to reproduce experimental B results rather accurately using the Tsonopoulos corresponding-states correlation, provided that the mixture-specific interaction parameter for this correlation is determined. Therefore, we concentrated our efforts on the search of ways to estimate this parameter. We found an empirical linear correlation between the interaction parameter and the Gibbs energy of hydration of a compound in water at 298 K, 0.1 MPa. Certainly, the Gibbs energy of hydration at ambient conditions is not a perfect measure of the extent of the attractive forces between water and a solute in the gas phase. However, pragmatically it is probably the best choice from possible single descriptors. In addition, data for normal alkanes from ethane to octane suggest that there is also a rather weak "size" dependence of the interaction parameter. There is also empirical evidence that a group contribution approximation is applicable to cross virial coefficients for interactions between water and members of homologous series of organic compounds.